

Lefschetz-thimble path integral for studying the Silver Blaze problem

Yuya Tanizaki

RIKEN BNL Research Center, BNL

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Collaborators: Yoshimasa Hidaka (RIKEN), Tomoya Hayata (Chuo Univ)

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Motivation: Sign problem, Silver Blaze problem

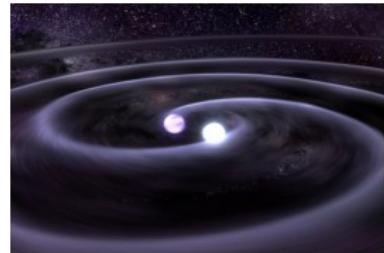
Sign problem of finite-density QCD

QCD

Fundamental theory for quarks and gluons

Neutron star

- Cold and dense nuclear matter
- $2m_{\text{sun}}$ neutron star (2010)
- Gravitational-wave observations (2016~)



Neutron star merger
(image from NASA)

Reliable theoretical approach to **equation of state** must be developed!

$$Z_{\text{QCD}}(T, \mu) = \int \mathcal{D}A \underbrace{\text{Det}(\not{D}(A, \mu_q) + m)}_{\text{quark}} \underbrace{\exp(-S_{\text{YM}}(A))}_{\text{gluon}}.$$

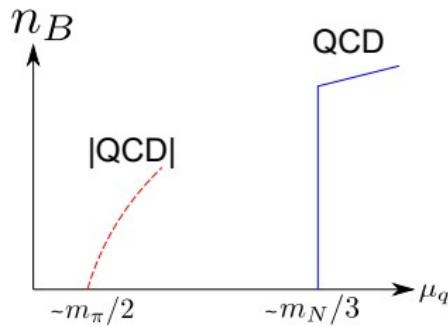
Sign problem: $\text{Det}(\not{D}(A, \mu_q) + m) \not\geq 0$ at $\mu_q \neq 0$.

Sign problem of finite-density QCD

QCD & $|QCD|$

$$Z_{\text{QCD}} = \int \mathcal{D}A (\det \not{D}) e^{-S_{\text{YM}}}, \quad Z_{|QCD|} = \int \mathcal{D}A |\det \not{D}| e^{-S_{\text{YM}}}.$$

If these two were sufficiently similar, we have no practical problems. However, it was observed in lattice QCD simulation that at $T = 0$ (e.g., Barbour et. al. (PRD **56** (1998) 7063))



Baryon Silver Blaze problem

The curious incident of the dog in the night-time (Holmes, Silver Blaze).

Problem: Show that $n_B = 0$ for $\mu_q < m_N/3$ using path integral.

(Cohen, PRL **91** (2003) 222001)

Current situation: For $\mu_q < m_\pi/2$, the problem is solved.

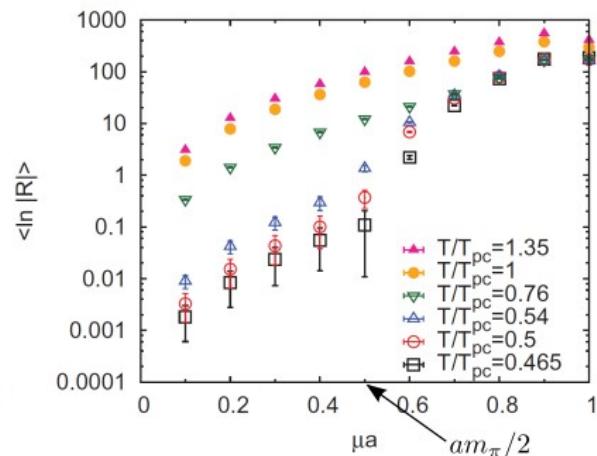
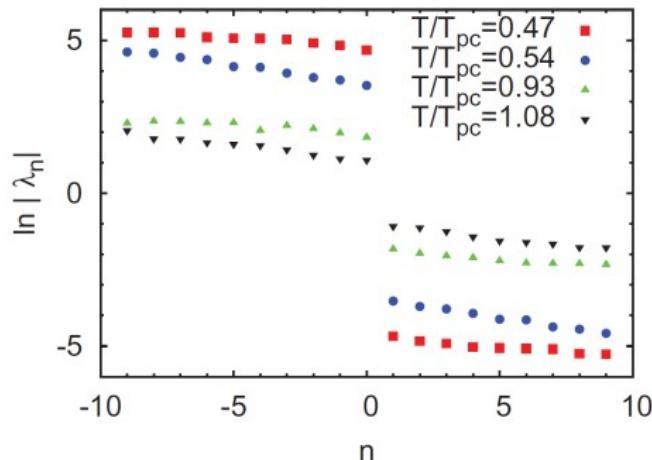
Quark det. is

$$\frac{\text{Det}(\not{D}(A, \mu_q) + m)}{\text{Det}(\not{D}(A, 0) + m)} \simeq \prod_{0 < \text{Re}(\lambda_A) < \mu_q} (1 + e^{-\beta(\lambda_A - \mu_q)}) ,$$

and $\text{ess-min}_A(\text{Re}(\lambda_A)) = m_\pi/2$. (Cohen, PRL **91** (2003) 222001,
 Adams, PRD **70** (2004) 045002, Nagata et. al., PTEP **2012** 01A103).

Spectrum of $\gamma_4(\not{D}_A + m)$

Gap of $\{\lambda\} = \text{Spec}(\gamma_4(\not{D}_A + m))$ gives the pion mass (Gibbs).



Lattice study of the quark spectrum and the Dirac determinant.

(Nagata et. al., PTEP 2012 01A103)

Method: Path integral on Lefschetz thimbles

Sign problem of path integrals

Consider the path integral:

$$Z = \int \mathcal{D}x \exp(-S[x]).$$

- $S[x]$ is real \Rightarrow No sign problem. Monte Carlo works.
- $S[x]$ is complex \Rightarrow Sign problem appears!

If $S[x] \in \mathbb{C}$, eom $S'[x] = 0$ may have **no** real solutions $x(t) \in \mathbb{R}$.

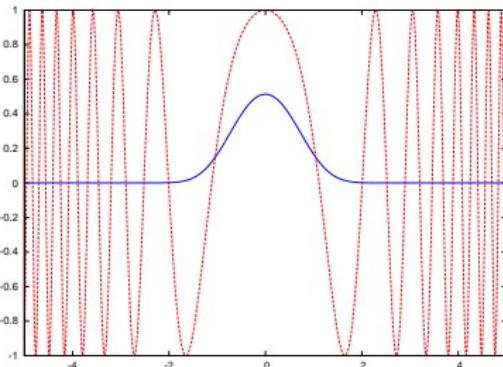
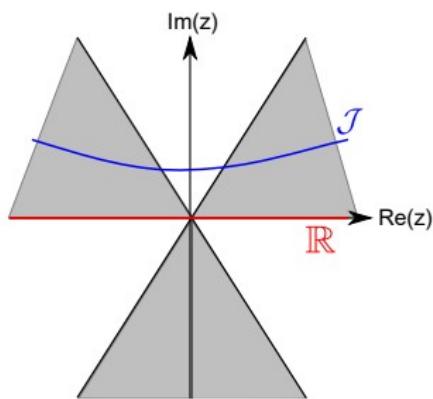
Idea: Complexify $x(t) \in \mathbb{C}$!

Lefschetz thimble for Airy integral

Airy integral is given as

$$\text{Ai}(a) = \int_{\mathbb{R}} \frac{dx}{2\pi} \exp i \left(\frac{x^3}{3} + ax \right)$$

Complexify the integration variable: $z = x + iy$.



Integrand on \mathbb{R} , and on \mathcal{J}_1
($a = 1$)

Rewrite the Airy integral

There exists two Lefschetz thimbles \mathcal{J}_σ ($\sigma = 1, 2$) for the Airy integral:

$$\text{Ai}(a) = \sum_{\sigma} n_{\sigma} \int_{\mathcal{J}_{\sigma}} \frac{dz}{2\pi} \exp i \left(\frac{z^3}{3} + az \right).$$

n_{σ} : intersection number of the steepest ascent contour \mathcal{K}_{σ} and \mathbb{R} .

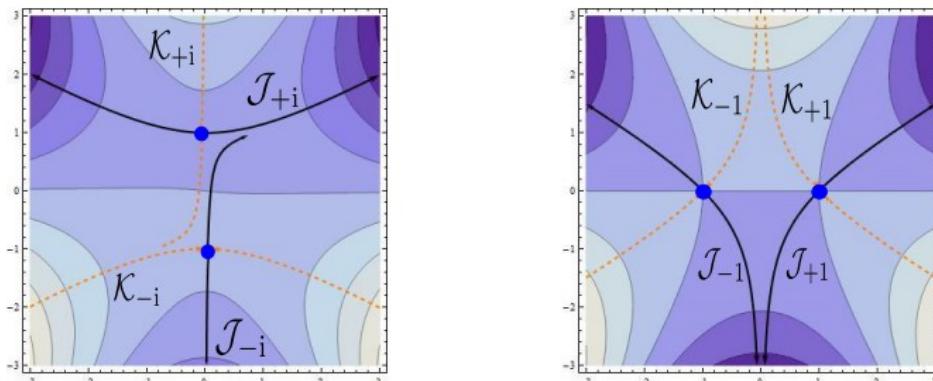


Figure: Lefschetz thimbles \mathcal{J} and duals \mathcal{K} ($a = 1e^{0.1i}, -1$)

Lefschetz decomposition formula

Oscillatory integrals with **many variables** can be evaluated using the “steepest descent” cycles \mathcal{J}_σ : (classical eom $S'(z_\sigma) = 0$)

$$\int_{\mathbb{R}^n} d^n x e^{-S(x)} = \sum_{\sigma} \langle \mathcal{K}_{\sigma}, \mathbb{R} \rangle \int_{\mathcal{J}_{\sigma}} d^n z e^{-S(z)}.$$

\mathcal{J}_σ are called Lefschetz thimbles, and $\text{Im}[S]$ is constant on it:

$$\mathcal{J}_\sigma = \left\{ z(0) \left| \lim_{t \rightarrow -\infty} z(t) = z_\sigma \right. \right\}, \quad \frac{dz^i(t)}{dt} = \overline{\left(\frac{\partial S(z)}{\partial z^i} \right)}.$$

$\langle \mathcal{K}_{\sigma}, \mathbb{R} \rangle$: intersection numbers of duals \mathcal{K}_{σ} and \mathbb{R}^n

($\mathcal{K}_{\sigma} = \{z(0) | z(\infty) = z_\sigma\}$).

[Witten, arXiv:1001.2933, 1009.6032]

[Christoforetti et al. (PRD(2012)), Fujii et al. (JHEP 1310), etc.]

Analysis: Semi-classical analysis of the one-site Hubbard model

One-site Fermi Hubbard model

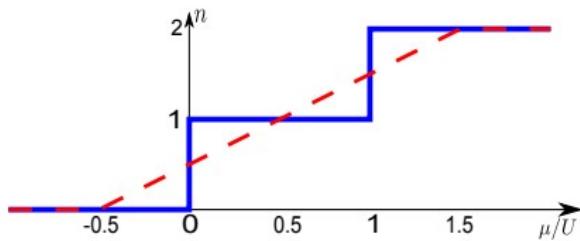
One-site Hubbard model:

$$\hat{H} = U\hat{n}_\uparrow\hat{n}_\downarrow - \mu(\hat{n}_\uparrow + \hat{n}_\downarrow).$$

Fock state gives the number density immediately:

$$\langle \hat{n} \rangle = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln Z = \frac{2(e^{\beta\mu} + e^{\beta(2\mu-U)})}{1 + 2e^{\beta\mu} + e^{\beta(2\mu-U)}}.$$

In the zero-temperature limit,



(YT, Hidaka, Hayata, 1509.07146)(cf. Monte Carlo with 1-thimble approx. gives a wrong result:

Fujii, Kamata, Kikukawa, 1509.08176, 1509.09141; Alexandru, Basar, Bedaque, 1510.03258.)

Path integral for one-site model

We consider the $(0 + 1)$ -dimensional fermion model,

$$S = \int_0^\beta d\tau \left(\frac{\varphi^2}{2U} + \psi^* [\partial_\tau + (-U/2 - \mu - i\varphi)] \psi \right).$$

The path-integral expression for the one-site Hubbard model:

$$Z = \sqrt{\frac{\beta}{2\pi U}} \int_{\mathbb{R}} d\varphi \underbrace{\left(1 + e^{\beta(i\varphi + \mu + U/2)}\right)^2}_{\text{Fermion Det}} e^{-\beta\varphi^2/2U}.$$

Integrand has complex phases causing the sign problem.

φ is an auxiliary field for the number density:

$$\langle \hat{n} \rangle = \text{Im}\langle \varphi \rangle / U.$$

Sign problem and fermion determinant

One-site Hubbard model:

$$\text{Det} \left[\partial_\tau - \left(\mu + \frac{U}{2} + i\varphi \right) \right] = (1 + e^{-\beta(-U/2-\mu)} e^{i\beta\varphi})^2.$$

Quark determinant in QCD:

$$\text{Det} [\gamma_4 (\not{D}_A + m) - \mu] = \mathcal{N}(A) \prod_{\varepsilon_j > 0} (1 + e^{-\beta(\varepsilon_j - \mu - i\phi_j)}) (1 + e^{-\beta(\varepsilon_j + \mu + i\phi_j)}),$$

where the spectrum of $\gamma_4 (\not{D}_A + m)$ is

$$\lambda_{(j,n)} = \varepsilon_j(A) - i\phi_j(A) + (2n+1)i\pi T.$$

Minimal value of $\varepsilon(A) = m_\pi/2$.

Silver Blaze problem for $\mu < -U/2$, $\mu < m_\pi/2$

One-site Hubbard model: As $\beta U \gg 1$ and $-U/2 - \mu > 0$,

$$\text{Det} \left[\partial_\tau - \left(\mu + \frac{U}{2} + i\varphi \right) \right] = \left(1 + e^{-\beta(-U/2-\mu)} e^{i\beta\varphi} \right)^2 \simeq 1.$$

The sign problem almost disappears, so that $\mathcal{J}_* \simeq \mathbb{R}$.

Finite-density QCD: As $\beta \rightarrow \infty$ and $\mu < m_\pi/2$,

$$\frac{\text{Det} [\gamma_4(\not{D}_A + m) - \mu]}{\text{Det} [\gamma_4(\not{D}_A + m)]} \rightarrow 1.$$

The sign problem disappears by the reweighting method.
 \Rightarrow Lefschetz thimbles \simeq Original integration regions

Flows at $\mu/U < -0.5$ (and $\mu/U > 1/5$)

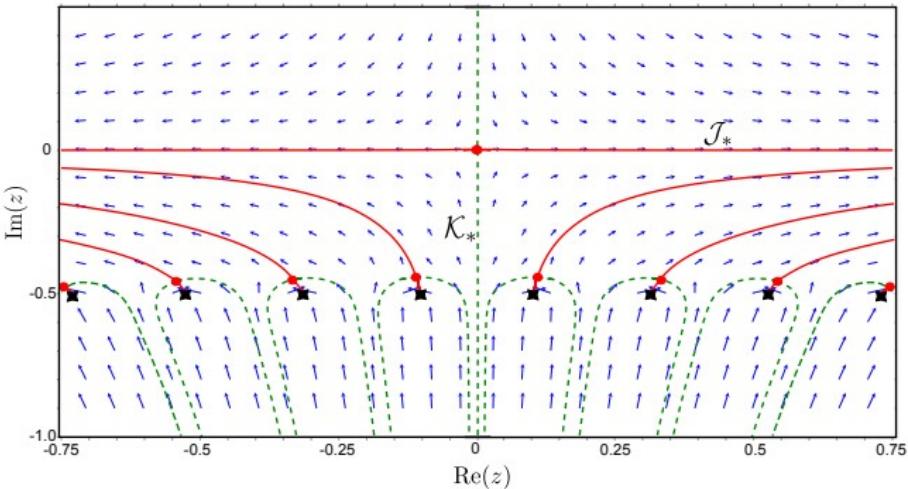


Figure: Flow at $\mu/U = -1$. $\mathcal{J}_* \simeq \mathbb{R}$.

$$Z = \int_{\mathcal{J}_*} dz e^{-S(z)}.$$

Number density: $n_* = 0$ for $\mu/U < -0.5$, $n_* = 2$ for $\mu/U > 1.5$.
 (YT, Hidaka, Hayata, 1509.07146)

Silver Blaze problem for $\mu > -U/2, \mu > m_\pi/2$

One-site Hubbard model: At each real config., the magnitude is exponentially large:

$$\text{Det} \left[\partial_\tau - \left(\mu + \frac{U}{2} + i\varphi \right) \right] = O(e^{\beta(U+\mu/2)})$$

This large contributions must be **canceled** exactly in order for $n = 0$.

Finite density QCD: The situation is almost the same, since

$$\frac{\text{Det}(\mathcal{D}(A, \mu_q) + m)}{\text{Det}(\mathcal{D}(A, 0) + m)} \simeq \prod_{\text{Re}(\lambda_A) < \mu_q} \exp \beta (\mu_q - \lambda_A),$$

but $n_B = 0$ for $\mu_q \lesssim m_N/3$.

Flows at $-0.5 < \mu/U < 1.5$

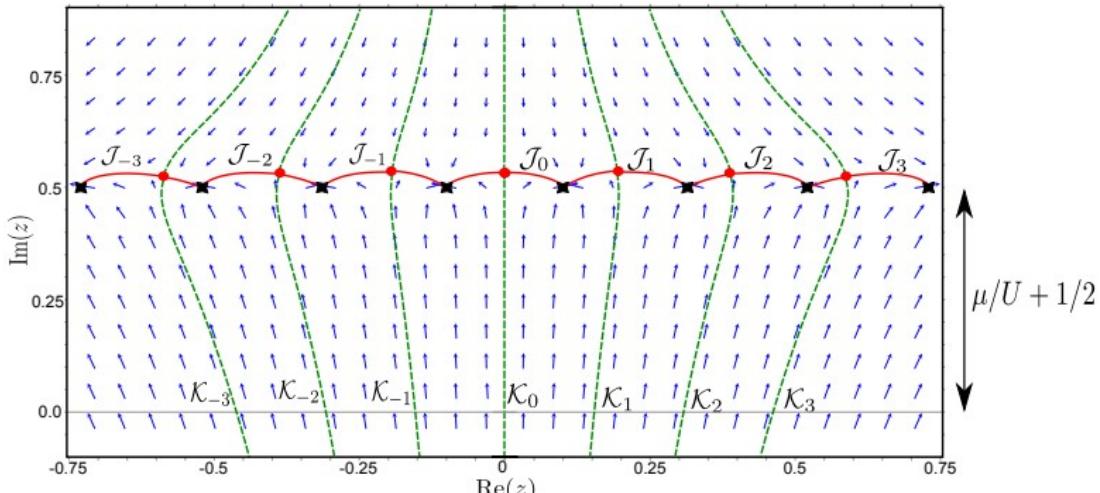


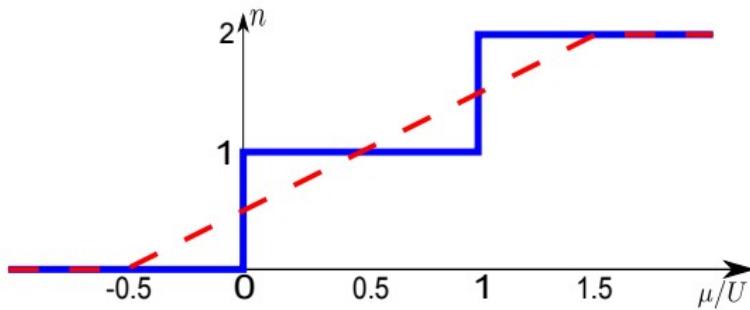
Figure: Flow at $\mu/U = 0$

Complex saddle points lie on $\text{Im}(z_m)/U \simeq \mu/U + 1/2$.

This value is far away from $n = \text{Im} \langle z \rangle/U = 0, 1, \text{ or } 2$.

Curious incident of n in one-site Hubbard model

We have a big difference bet. the exact result and naive expectation:



This is similar to what happens for QCD and |QCD|.

$$\mu/U = -0.5 \Leftrightarrow \mu_q = m_\pi/2.$$

Complex classical solutions

If $\beta U \gg 1$, the classical sol.
for $-0.5 < \mu/U < 1.5$
are labeled by $m \in \mathbb{Z}$:

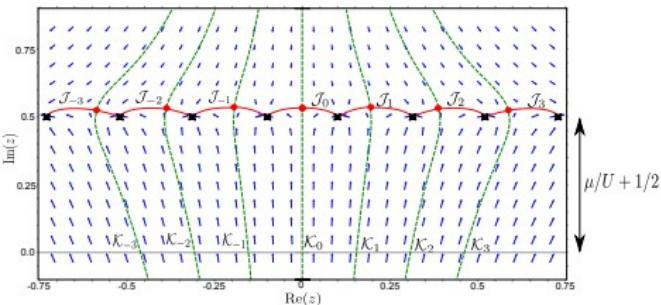
$$z_m \simeq i \left(\mu + \frac{U}{2} \right) + 2\pi m T.$$

At these solutions, the classical actions become

$$S_0 \simeq -\frac{\beta U}{2} \left(\frac{\mu}{U} + \frac{1}{2} \right)^2,$$

$$\text{Re}(S_m - S_0) \simeq \frac{2\pi^2}{\beta U} m^2,$$

$$\text{Im } S_m \simeq 2\pi m \left(\frac{\mu}{U} + \frac{1}{2} \right).$$

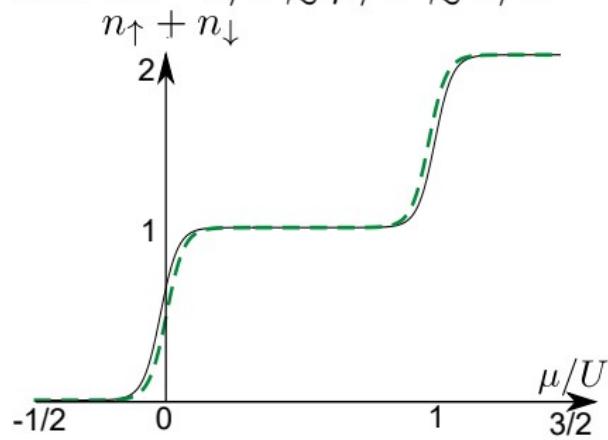


Semiclassical partition function

Using complex classical solutions z_m , let us calculate

$$Z_{\text{cl}} := \sum_{m=-\infty}^{\infty} e^{-S_m} = e^{-S_0(\mu)} \theta_3 \left(\pi \left(\frac{\mu}{U} + \frac{1}{2} \right), e^{-2\pi^2/\beta U} \right).$$

This expression is valid for $-1/2 \lesssim \mu/U \lesssim 3/2$.



Important interference among multiple thimbles

Let us consider a “phase-quenched” multi-thimble approximation:

$$Z_{|\text{cl.}|} = \sum_m |e^{-S_m}| = e^{-S_0(\mu)} \theta_3(0, e^{-2\pi^2/\beta U}).$$

- Lee–Yang zeros cannot appear at $\mu/U = 0, 1$.
- One-thimble, or “phase-quenched”, result: $n \simeq \mu/U + 1/2$.

Consequence

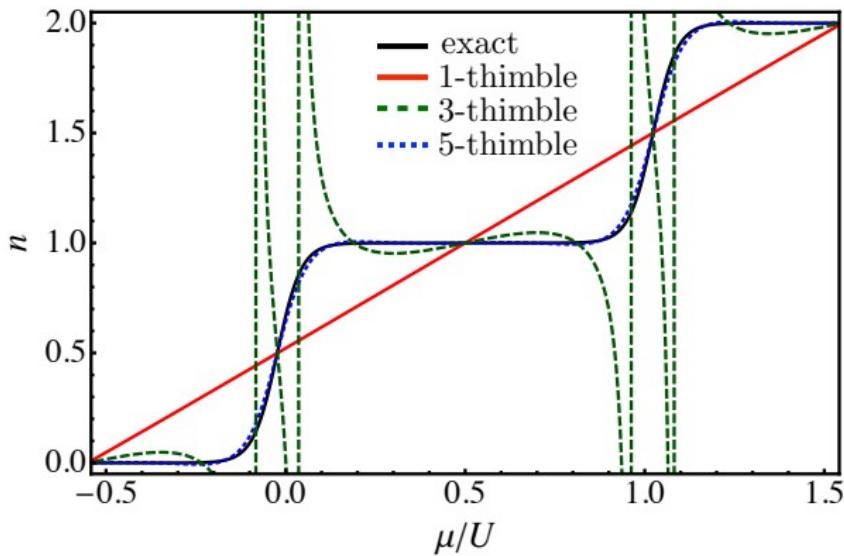
To understand the Silver Blaze problem, we need interference of complex phases among different Lefschetz thimbles.

(cf. Particle Productions: Dumulu, Dunne, PRL 104 250402)

(cf. Hidden Topological Angles: Behtash, Sulejmanpasic, Schäfer, Ünsal, PRL 115 041601)

Numerical results

Results for $\beta U = 30$: (1, 3, 5-thimble approx.: \mathcal{J}_0 , $\mathcal{J}_0 \cup \mathcal{J}_{\pm 1}$, and $\mathcal{J}_0 \cup \mathcal{J}_{\pm 1} \cup \mathcal{J}_{\pm 2}$)



Necessary number of Lefschetz thimbles $\simeq \beta U / (2\pi)$.

(YT, Hidaka, Hayata, NJP 18 (2016) 033002, arXiv:1509.07146[hep-th])

Bonus: Complex Langevin method

Complex Langevin method

Complex Langevin has been regarded as a sign-problem solver via stochastic quantization (Klauder, PRA 29, 2036 (1984), Parisi, PLB 131, 393 (1983)):

$$\frac{dz_\eta(\theta)}{d\theta} = -\frac{\partial S}{\partial z}(z_\eta(\theta)) + \sqrt{\hbar}\eta(\theta).$$

θ : Stochastic time, η : Random force $\langle \eta(\theta)\eta(\theta') \rangle_\eta = 2\delta(\theta - \theta')$.

Properties:

- Numerical cost is very cheap.
- Ito calculus shows $\langle O(z_\eta(\infty)) \rangle_\eta$ solve the Dyson–Schwinger eq.
- Sign problem does not appear.
- But, it fails in some cases. \Rightarrow When does it fail?

Semiclassical incorrectness of CL method

If \hbar is small enough, we can show a sufficient condition for incorrect behaviors of CL method.

(Hayata, Hidaka, YT, 1511.02437)

Assume that CL method is correct to derive the contradiction, then

$$\begin{aligned}\langle O(z_\eta) \rangle_\eta &\stackrel{!}{=} \int dx e^{-S(x)/\hbar} O(x) \\ &= \frac{1}{Z} \sum_{\sigma} \langle \mathcal{K}_\sigma, \mathbb{R}^n \rangle \int_{\mathcal{J}_\sigma} dz e^{-S(z)/\hbar} O(z).\end{aligned}$$

Since $\hbar \ll 1$,

$$\exists c_\sigma \geq 0 \quad \text{s.t.} \quad \langle O(z_\eta) \rangle_\eta \simeq \sum_{\sigma} c_\sigma O(z_\sigma).$$

Semiclassical inconsistency

In the semiclassical analysis, one now obtains (for dominant saddle points)

$$c_\sigma = \frac{\langle \mathcal{K}_\sigma, \mathbb{R}^n \rangle}{Z} \sqrt{\frac{2\pi\hbar}{S''(z_\sigma)}} e^{-S(z_\sigma)/\hbar}.$$

The right hand side can be complex, which **contradicts** with $c_\sigma \geq 0!$
 (Hayata, Hidaka, YT, 1511.02437)

We show that the complex Langevin is wrong if

- There exist several dominantly contributing saddle points, and
- Those saddle points have different complex phases.

Proposal for modification

Assume as a working hypothesis that

$$c_\sigma = \frac{\langle \mathcal{K}_\sigma, \mathbb{R} \rangle}{Z} \left| \sqrt{\frac{2\pi\hbar}{S''(z_\sigma)}} e^{-S(z_\sigma)/\hbar} \right|.$$

Because of the localization of probability distribution P , it would be given as

$$P = \sum_{\sigma} c_{\sigma} P_{\sigma}, \quad \text{supp}(P_{\sigma}) \cap \text{supp}(P_{\tau}) = \emptyset.$$

Assumption means “CL = phase quenched multi-thimble approx.”:

$$\langle O(z_\eta) \rangle_\eta \simeq \sum_{\sigma} \frac{\langle \mathcal{K}_\sigma, \mathbb{R} \rangle}{Z} \left| \sqrt{\frac{2\pi\hbar}{S''(z_\sigma)}} e^{-S(z_\sigma)/\hbar} \right| O(z_\sigma).$$

Proposal for modification (cont.)

If so, defining the phase function

$$\Phi(z, \bar{z}) = \sum_{\sigma} \sqrt{\frac{|S''(z_{\sigma})|}{S''(z_{\sigma})}} e^{-i \operatorname{Im} S(z_{\sigma})/\hbar} \chi_{\operatorname{supp}(P_{\sigma})}(z, \bar{z}),$$

we can compute

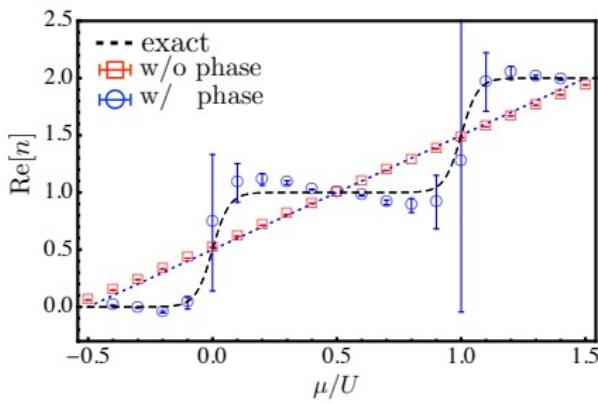
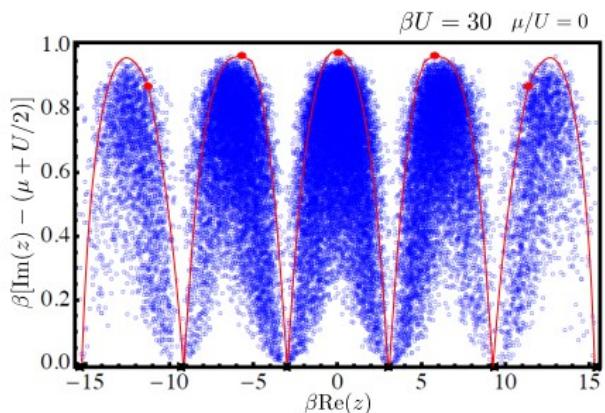
$$\langle O(z_{\eta}) \rangle^{\text{new}} := \frac{\langle \Phi(z_{\eta}, \bar{z}_{\eta}) O(z_{\eta}) \rangle_{\eta}}{\langle \Phi(z_{\eta}, \bar{z}_{\eta}) \rangle_{\eta}}.$$

This new one is now consistent within the semiclassical analysis.

(Hayata, Hidaka, YT, arXiv:1511.02437[hep-lat])

Caution: Our proposal evades inconsistency, but is not necessarily correct. Can we improve the proposal?

Complex Langevin study of one-site fermion model



(Hayata, Hidaka, YT, 1511.02437)

Complex Langevin method cannot study the Silver Blaze problem of this model without introducing the reweighting procedure.

Summary and Conclusion

- Picard–Lefschetz theory gives a suitable framework for saddle-point analysis even if $S(\phi)$ takes complex values.
- One-site Hubbard model is a nice toy model to play with the sign problem.
- Destructive and constructive interference of complex phases among Lefschetz thimbles play a pivotal role for the baryon Silver Blaze.